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Description of Codes and Models to be Used in Risk Assessment

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FOREWORD

A Risk Assessment Modeling Committee was formed to exchange experiences and opinions relating to the use of numerical models for risk assessment. The committee included representatives from the U.S. Environmental Protection Agency, the Washington State Department of Ecology, the U.S. Department of Energy, and their contractors. In general, the committee meetings have enhanced understanding between the involved parties and hopefully improved the decision-making process. Continuation of the committee is recommended for completion of future milestones related to modeling, selection of additional computer codes, and to address computer code and modeling issues that arise during implementation of remedial investigation/feasibility study activities.

While opinions expressed by all members of the committee have been considered, this document does not necessarily reflect the views of individual committee members. Final selection of the computer codes recommended for use was performed by the Hanford Site Operations Contractor, Westinghouse Hanford Company. This recommendation is contained herein and provided to the U.S. Department of Energy to fulfill the M-29-01 Milestone: "Descriptions of Codes and Models to be Used in Risk Assessment."

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1.0 INTRODUCTION

1.1 PURPOSE

Human health and environmental risk assessments will be performed as part of the Comprehensive Environmental Response, Compensation, and Liability Act of 1980 (CERCLA) remedial investigation/feasibility study (RI/FS) activities at the Hanford Site. Analytical and computer encoded numerical models are commonly used during both the remedial investigation (RI) and feasibility study (FS) to predict or estimate the concentration of contaminants at the point of exposure to humans and/or the environment. For the purposes of this discussion, the term "computer code" or "software" will refer to the list of computer commands that perform mathematical calculations and manipulate data, while the term "model" will refer to the combination of data and computer code that represents or describes a physical system. This document has been prepared to identify the computer codes that will be used in support of RI/FS human health and environmental risk assessments at the Hanford Site. In addition to the CERCLA RI/FS process, it is recommended that these computer codes be used when fate and transport analyses is required for other activities. Additional computer codes may be used for other purposes (e.g., design of tracer tests, location of observation wells, etc.).

This document provides guidance for unit managers in charge of RI/FS activities. Use of the same computer codes for all analytical activities at the Hanford Site will promote consistency, reduce the effort required to develop, validate, and implement models to simulate Hanford Site conditions, and expedite regulatory review. Although creating guidelines for computer codes at the Hanford Site is intended to limit the number of codes used at the Hanford Site, it should not discourage advancements in modeling capability or use of alternative software when warranted. It is recognized that software development is a dynamic process and periodic upgrading will be necessary as better computer codes are developed. Furthermore, unique situations may arise that could be better modeled using software not included in these guidelines.

This document is divided into four section: (1) Introduction, (2) Discussion, (3) Selection Criteria, and (4) Recommendations. The "Discussion" section provides a description of how models will likely be developed and utilized at the Hanford Site. It is intended to summarize previous environmental-related modeling at the Hanford Site and provide background for future model development. The "Selection Criteria" section lists the modeling capabilities that are desirable for the Hanford Site and compares the codes that were proposed for consideration. Only those codes that have been used at the Hanford Site were evaluated. The "Recommendations" section lists the codes proposed to support future risk assessment modeling at the Hanford Site, and provides the rational for the codes selected.

1.2 SCOPE

The specific objective of this document is to satisfy the M-29-01 Milestone of the Hanford Federal Facility Agreement and Consent Order, referred to as the Tri-Party Agreement (Ecology et al. 1989). The direction of this milestone was to "Identify and Submit Descriptions of Codes and Models to be Used in Risk Assessment." A follow-up document will satisfy the requirements of the M-29-02 Milestone, which requires "a plan for development of area wide groundwater models to support risk assessment and to evaluate impacts of changing groundwater flow fields." The third and final milestone (M-29-03) requires a preparation of a risk assessment methodology document. A risk assessment committee is guiding the completion of the third milestone. The first two milestones are support documents for the third milestone.

A model is defined as a simplified description of a physical system. When considering human health and environmental risk assessments, the physical system is defined to include the waste site, the environmental setting, and the pathway to the potential receptors. This document is limited to modeling of the release and transport of contaminants from the waste site to the receptor via the air, surface water, and groundwater. Milestone M-29-03 will address the development of a risk assessment methodology that includes modeling of dose and response of the potential receptors. A variety of models, ranging from simplified analytical models to complex computer-encoded numerical models, are available for modeling the fate and transport of contaminants, i.e., prediction of contaminant concentrations in air, surface water, and groundwater. The selection of appropriate models depends on several site-specific factors, including (but not limited to) the nature and extent of contamination, spatial geometry, complexity of the physical system, presence of an exposed population, points of compliance, space and time scales, and extent of site characterization. The primary use of these models will be to predict the concentrations of various contaminants in the air, soil, groundwater, and surface water.

This document reflects an emphasis on the subsurface pathway, specifically unsaturated and saturated groundwater transport. The subsurface pathway was considered more important at this point in time because the vast majority of contaminants at the Hanford Site are found in the soil and groundwater and transport in the subsurface will require evaluation in all cases beginning with the baseline risk assessment or no-action alternative. All proposed remedial actions will be compared to the results from this analysis. Other pathways, including air and surface water, may require more focused consideration in the future depending on the method and level of remediation considered.

Moreover, this document does not address the use of analytical models, waste package models, or geochemical models. Although analytical models are expected to play an important role for preliminary evaluation, they are not included here because they are generally abundant, require little development, and are easy to use, review, and test. Although both waste package and geochemical models may be important for confirmation of field or laboratory observations, it is believed that their use will be infrequent and will be addressed on a case-by-case basis.

2.0 DISCUSSION

This section sets the stage for how models will likely be developed and utilized in support of risk assessments. Model development will be specifically addressed in the M-29-02 Milestone. The discussion provides the background for Section 3.0 (Selection Criteria) and Section 4.0 (Recommendations).

2.1 MODELING FRAMEWORK

A framework for screening and defining the need for contaminant fate and transport modeling in air, surface water, and groundwater has been prepared by the U.S. Environmental Protection Agency (EPA [EPA 1988]) and is shown in Figure 2-1 for air, Figure 2-2 for surface water, and Figure 2-3 for soils and groundwater. It is recommended that these decision networks be used during the planning process to help structure the RI/FS process and determine the need for and nature of contaminant transport modeling. The following guidelines are proposed:

1) The complexity of the model should be consistent with the objectives of the risk assessment.

   Calculations using simple analytical models may be sufficient for preliminary evaluation, while more complex numerical models may be required for determining the final Record of Decision (ROD). It is expected that detailed numerical modeling will be performed when simpler models reveal the potential for violating standards of safe exposure or health risk. When contaminant inventory is small, the waste form is extremely stable and/or the constituents are relatively benign, the amount of risk may be many orders of magnitude less than allowable standards. Alternatively, in situations where large quantities of relatively toxic constituents are free to migrate, the risk may be clearly unacceptable. Simple analytical models will be relied upon to identify these situations, thereby significantly reducing the time and resources that would be expended if extensive numerical modeling were performed for all situations. This screening approach is analogous to the multi-tired approach recommended by the EPA (EPA 1988). More sophisticated modeling may be necessary to compare remedial alternatives at high risk sites.

   Furthermore, if it is anticipated that detailed modeling will eventually be required, it may be more efficient to begin development of a more powerful numerical model during the early screening stages of risk assessment. The decision between using the initial simple analytical codes or the more powerful numerical codes will be carefully weighed on a case-by-case basis. Input from the regulators is encouraged during screening assessments to help identify the appropriate level of modeling for use in analyses supporting the anticipated ROD.

2) Use of models will be factored into the RI/FS process during the planning stages and considered throughout the RI/FS process.

   During the initial planning process, numerical modeling will be useful to help structure the conceptual model of the physical system, identify potential migration pathways and points of exposure, and to define data needs. During the investigation phase of the RI/FS, modeling will provide a means for interpreting data, revising the conceptual model, and determining if sufficient data have been collected. Additionally, models will be used to provide information for the baseline risk assessment. The FS process will rely on models to estimate the effectiveness, efficiency, economy, and risk posed by the various remediation and mitigation approaches. It is, therefore, important that the proper model be selected and appropriate data is collected in the RI/FS.

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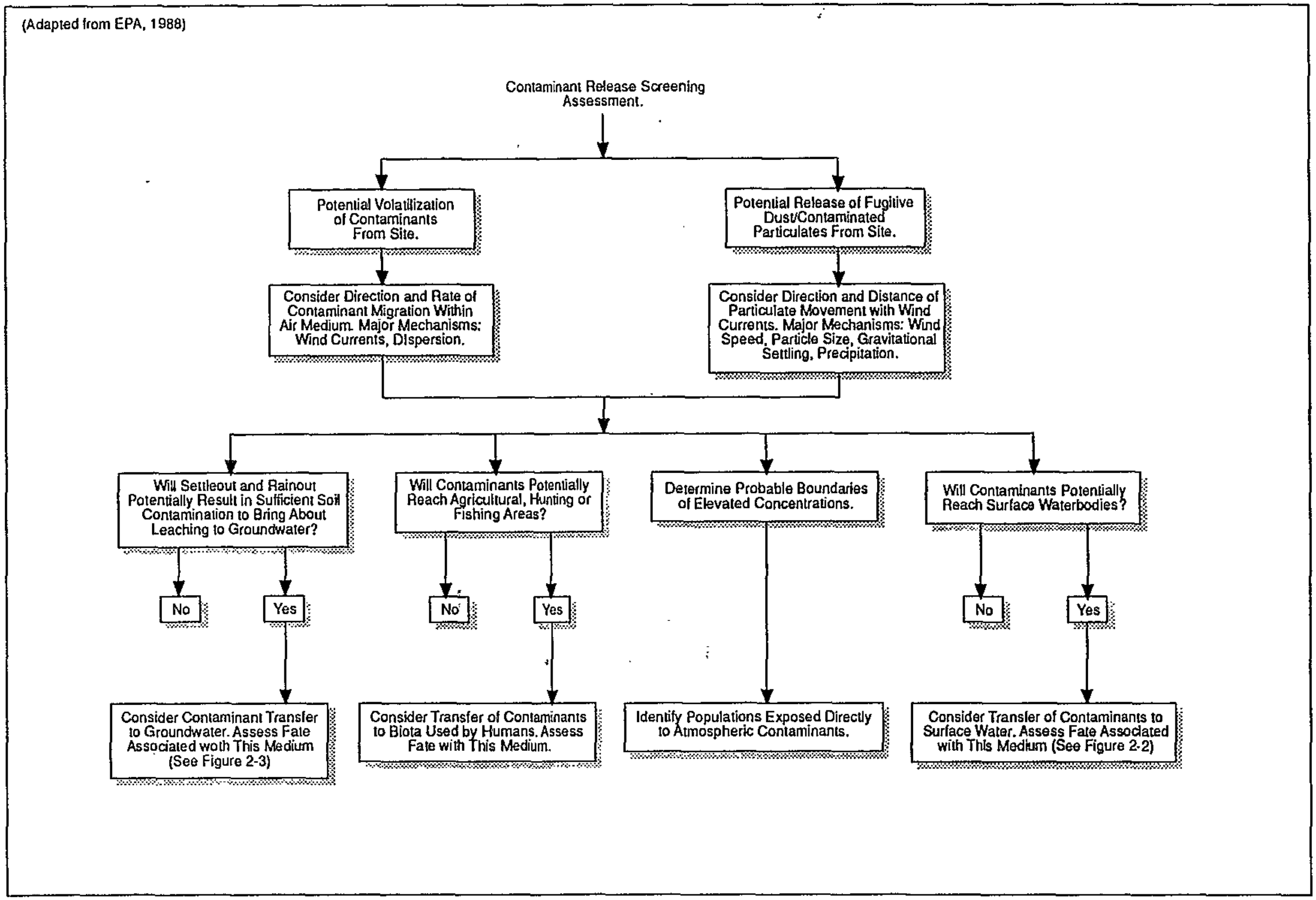

Figure 2-1. Environmental Fate Screening Assessment Decision Network: Atmosphere.

(Adapted from EPA, 1988)

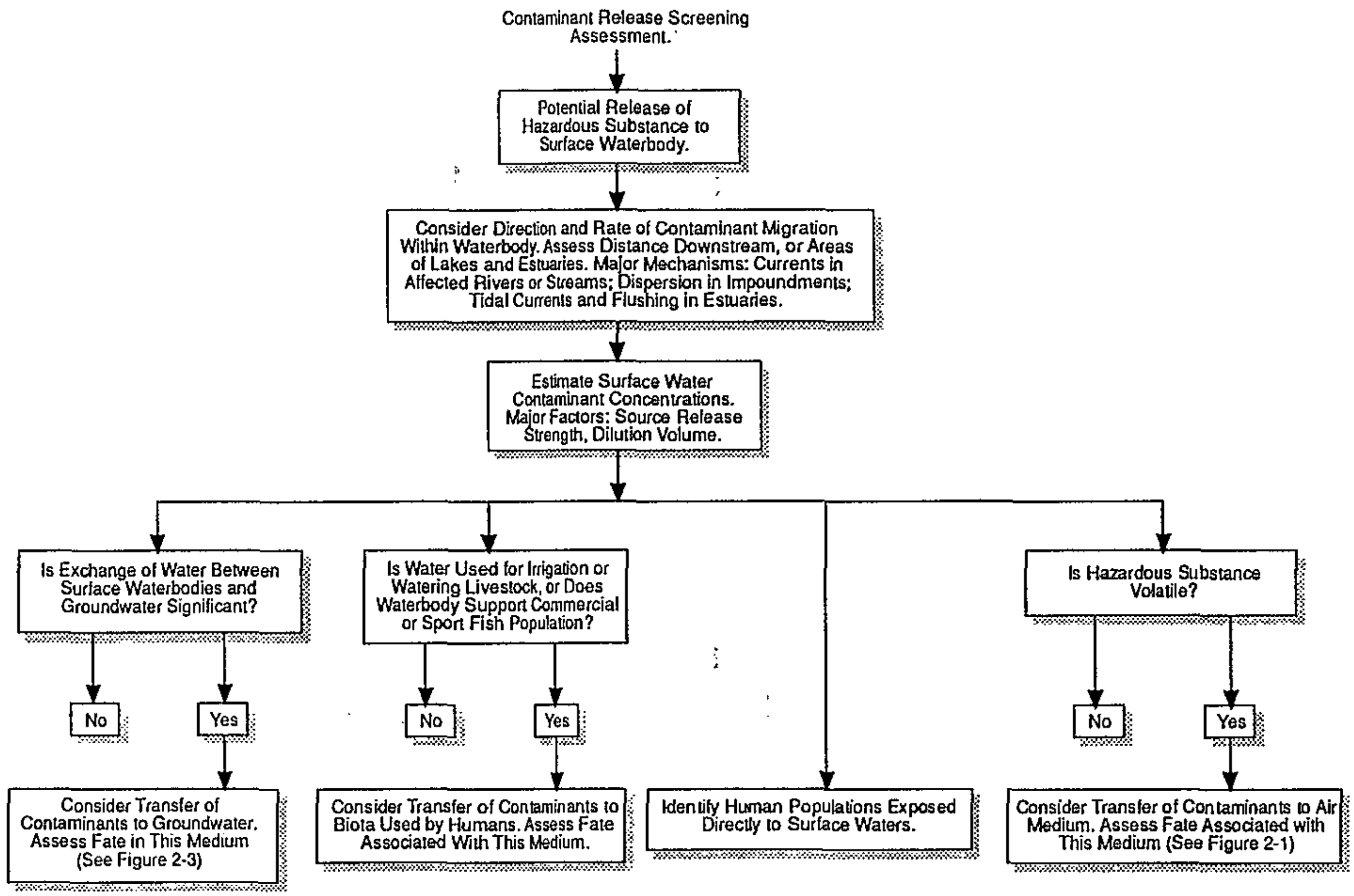

Figure 2-2. Environmental Fate Screening Assessment Decision Network: Surface Water.

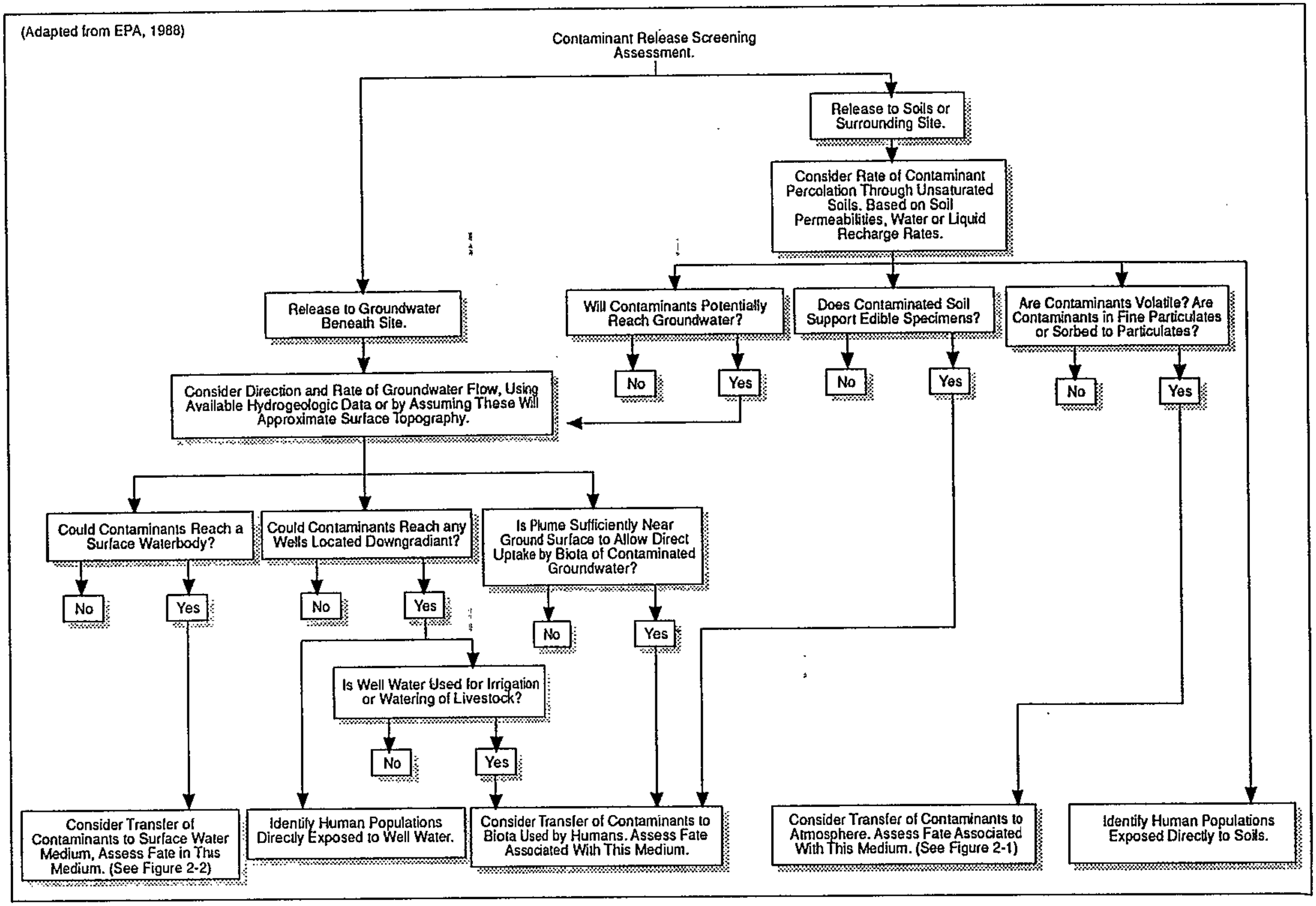

Figure 2-3. Environmental Fate Screening Assessment Decision Network: Soils and Groundwater.

3) Modeling efforts associated with remediation of various waste units at the Hanford Site (waste sites, operable units, aggregate areas) will be coordinated to ensure consistency and transferability of data and results, thereby minimizing total effort.

It is likely that different RI/FS efforts will utilize overlapping or similar models. The characteristics of these models, including general conceptual elements, flow and transport parameters, boundary conditions, and level of complexity should be consistent. Encouragement of such consistency begins with the selection of a standard set of codes and the coordinated development and application of models that use these codes.

4) Improvements in modeling capabilities will be encouraged.

The future may bring improvements in modeling capabilities, and the list of Hanford Site software should evolve to incorporate these technical advances. Changes to the list of Hanford Site software will be based on demonstrated need and undertaken with the consensus of both the technical and regulatory communities.

5) Use of software for risk assessments not included in this document will be allowed given sufficient technical justification.

It is conceivable that situations will arise requiring software capabilities not included in the Hanford Site list of codes. If this occurs, it may be technically justifiable to utilize a computer code that includes the necessary capability even if it is not on the Hanford Site list. Suggested guidelines for approval of new software are provided in Section 4.5.

6) Uncertainty and parameter sensitivity will be qualified with nonprobabilistic approaches.

An evaluation that includes the quantification of uncertainty will be required in most situations. Complete understanding and description of natural hydrogeologic systems is not possible; therefore, model uncertainty is unavoidable given limitations in data collection, modeling capability, and theoretical simplifications. Furthermore, in most situations it is important to know the sensitivity of model results to variations in model parameters. Although uncertainty and parameter sensitivity could be quantified with probabilistic approaches, sufficient data may not be available to provide statistically defensible results. In such cases, nonprobabilistic approaches (such as manual variation of parameters using deterministic models) will allow qualitative assessment of prediction uncertainty. The data needed to quantify estimates of uncertainty and parameter sensitivity will be determined as part of the RI/FS through the establishment of data quality objectives.

2.2 MODEL DEVELOPMENT PROCESS

Model development should continue throughout the RI/FS process in response to new data, improved data interpretation, changing exposure assessment needs, and other factors. A more complete description of the model development process will be provided in the milestone (M-29-02) that will address the development of area-wide models. However, the initial stages of model development are summarized below to illustrate how the needs of the project might affect the selection and application of computer codes.

1) Identify objectives

All modeling activities should begin with a clear definition of the project objectives. This definition is important because it affects the choice of computer codes, the data needs, the density of the spatial grid, and the effort involved. Future objectives should also be considered during model development.

2) Evaluate existing data

Initial model development will rely on readily available data. Attention will be focused on parameters that have the most impact on predicted concentrations. If data are lacking, it may be necessary to assume values and provide rationale for these assumptions.

3) Define the appropriate conceptual model

Available data will be synthesized into a coherent depiction of the physical system, referred to as a conceptual model. The conceptual model may address a single component or multiple components, including the waste source, the engineered barriers, the surrounding hydrogeologic system, and the potential exposure pathways. Determining which components to include in the model depends on the modeling objectives and the existing understanding of the physical system.

4) Select the appropriate analytical or numerical model

The modeling effort should utilize a level of sophistication that is appropriate considering the modeling objectives, the available data, the complexity of the conceptual model, and the required accuracy of the results. If a numerical model is used, the spatial grid must also be defined at this stage. The ability to address future modeling needs and incorporate future data may affect the choice of models.

5) Incorporate data into the mathematical model and identify additional data needs.

This stage of model development requires representation of actual or estimated data as parameters or boundary conditions in the mathematical model. For groundwater modeling, aquifer geometry and stratigraphy from borehole logs and geophysical surveys will be used to define the model boundaries, and measurements of hydraulic characteristics from aquifer tests and laboratory analyses will help determine parameters used in the model. Additional data needs should be identified during this stage.

6) Model calibration

Model calibration involves adjusting hydrogeologic structure, boundary conditions, and aquifer hydraulic parameters until simulated results compare well with observed conditions. For groundwater flow models, calibration may include comparison of observed hydraulic head and gradient conditions with simulated results and comparison of observed plume velocities with simulated velocities.

Generally, the model should be calibrated using data that supports the primary process of interest. For example, if the model is used primarily to simulate flow and transport, then the model should be calibrated using information on flow (i.e., velocities from tracer studies, etc.) as opposed to an indirect measure such as the calibration against piezometric head variation.

Observations of actual conditions and behavior may not be readily available for characteristically long-term processes, such as vadose zone flow, diffusion from vitrified blocks, and transport of strongly sorbed constituents. For these processes, when no transport data exists, calibration may be difficult or impossible. In such case, it may be possible to bound the behavior, e.g., generally, it is accepted that areal recharge across the Hanford Site averages less than several inches per year.

2.3 PREVIOUS ENVIRONMENTAL TRANSPORT MODELING AT HANFORD

This section provides a summary of computer code development and use at the Hanford Site that supports environmental fate and transport modeling. For the most part, discussion is limited to recent experience that is important with regards to risk assessments and waste isolation performance assessments. This discussion provides a basis for the selection of computer codes and the recommendations found in Section 4.0.

2.3.1 Air

The development of air transport models for use at the Hanford Site was initiated in the 1940's. This activity was originally supported by the Atomic Energy Commission (AEC). The release of airborne contamination (gaseous and particulate emissions) from the stacks of various production facilities has long been recognized as a potential threat to human health and the environment. The basic models to predict transport and dispersion of airborne contaminants that are commonly in use today at the Hanford Site and across the country were derived from pioneering efforts performed under the auspices of the AEC. As a result, there is considerable confidence in these models for predicting the fate and transport of airborne contaminants at the Hanford Site.

Routinely used computer codes supporting Hanford Site operations include GENII and AIRDOS. Both models are used to calculate dose from the interaction of receptors and airborne radioactivity. The air transport model included in GENII is an atmospheric dispersion model that does not take into consideration depletion of air concentrations through deposition or scavenging (Napier et al. 1988). The atmospheric transport model included in GENII is an analytical solution to the multi-dimensional Gaussian diffusion model for continuous release. This analytical methodology is similar to the approach described in the EPA "Superfund Exposure Assessment Manual" (EPA 1988). In contrast to GENII, the atmospheric transport model contained in AIRDOS-PC allows for depletion resulting from the deposition and scavenging of radioactive contaminants (EPA 1989).

Although other more specialized computer codes, such as the Industrial Source Complex (ISC) model, have been used and are available for future use in support of health risk assessments, they have not been used routinely at the Hanford Site. The ISC is designed to address health hazards associated with hazardous chemicals from multiple sources.

2.3.2 Surface Water

The development of surface water models for application at the Hanford Site was initiated during the mid 1960's. Over the years, large quantities of heated effluent from the production reactors in the 100 Areas were discharged directly into the Columbia River. The COLHEAT computer code was developed to predict the fate of heated effluent discharged into the Columbia River (HEDL 1972). Thermographs were installed along the Columbia River beginning in the late 1960's and the temperature records from this network of thermographs were used routinely to calibrate the COLHEAT model. The COLHEAT computer code was used and maintained through the mid-1970's.

A mathematical model to simulate the transport of sediment and radioactivity in the Columbia River was developed in the mid-1970's (Onishi 1977). The resulting computer code (SERATRA) was used in a pilot-scale study to model the longitudinal and vertical distribution of sediments in the Columbia River between Priest Rapids and McNary dams. Sediment and radionuclide interactions and transport were investigated for three sediment fractions, (sand, silt, and clay). Although the preliminary results from the pilot-scale study were encouraging, the model was never used on a routine basis to simulate the transport of sediments and sediment-contaminant interactions in the Columbia River. Although the SERATRA computer code was not used to simulate sediment-contaminant transport in support of Columbia River studies, the code has been used successfully at other locations (Onishi et al. 1982).

The DWOPER computer code has been applied by the U.S. Army Corps of Engineers and the U.S. Bureau of Reclamation to simulate river stage variation in the Hanford Reach of the Columbia River (Fread 1973). The DWOPER code does not address contaminant transport.

2.3.3 Soil and Groundwater

A generic model of the mechanisms that generally influence the modeling of flow and transport of contaminants in the soil and groundwater system is shown in Figure 2-3. These mechanisms include; the release of contaminants to the soils and groundwater that surround the waste site, infiltration of groundwater beyond the root zone, migration of contaminants in partially saturated sediments, migration of contaminants in saturated sediments, multi-phase flow, and geochemistry. A brief description of the history of modeling these processes at the Hanford Site is discussed in the following sections.

2.3.3.1 Release Models. Contaminants find their way into the soil column through planned or accidental releases (spills or leaks), or through waste form degradation. The release of contaminants from specific waste forms rely on knowledge of the chemical and physical processes that govern degradation. With the great variety of wastes and waste containment systems that exist at the Hanford Site, a corresponding range of releases is envisioned. As a result, modeling of waste form release can be achieved by either of two methods: (1) simple, yet conservative models can be used in an attempt to bound the release, or (2) release can be quantified empirically through direct measurement. In support of the Hanford Defense Waste-Environmental Impact Statement (HDW-EIS) (DOE 1987), relatively simple conservative models were used to estimate the release from the various waste forms. Simulated waste forms have been studied in the laboratory to quantify the release from large monolithic grouted waste vaults proposed for use at the Hanford Site (Serne 1990). In either case, it is assumed that the release can be characterized and quantified as a boundary condition (contaminant concentration or mass flux) or initial condition for inclusion into the transport model. As such, it is proposed that contaminant release be addressed on a case-by-case basis depending on the specifics of the waste and waste site being assessed.

2.3.3.2 Infiltration Model. The ROD issued for the HDW-EIS (DOE 1987) identified the need for a better understanding on the mechanisms governing the rate of surface infiltration and percolation of water in the partially saturated sediments. Since that time, considerable emphasis has been placed on the quantification and development of analytical and numerical methods that can be used to predict the infiltration of water through partially saturated sediments at the Hanford Site. UNSAT-H has been developed for use at the Hanford Site and reflects the current state-of-the-art understanding of Hanford Site conditions (Fayer and Jones 1990). This computer code simulates the one-dimensional, non-isothermal, dynamic processes of infiltration, drainage, moisture redistribution, evaporation, and plant uptake of water. To date, calibration of the model has been limited to application of results from controlled lysimeter studies and experiments involving bare (nonvegetated) soils. Therefore, the model has not been uniformly calibrated to all conditions that exist across the Hanford Site.

2.3.3.3 Unsaturated Flow and Transport Model. Modeling of groundwater flow in the partially saturated sediments began in the mid 1960's. Over the years, a number of computer codes were developed and applied at the Hanford Site. The primary motivation stemmed from interest in studying single-shell tank releases, and the potential migration of contaminants through the thick zone of partially saturated sediments beneath the 200 Areas. The vadose zone is between 60 and 80 meters thick in these areas. To support the HDW-EIS, a simplified methodology for vadose zone flow simulation was described that relied on the assumption of unit hydraulic gradient conditions and application of the steady-state solution to the Richards' equation (DOE 1987). Recently, vadose zone analyses have been supported through the use of more sophisticated models, including PORFLO-3 (Sager and Runchal 1990), VAM2DH (Huyakorn et al. 1988), VAM3DCG (Huyakorn and Panday 1990) and TRACR3D (Travis 1984). PORFLO-3 has been used on a number of projects, including: (1) modeling the flow of liquid effluent from the 1324 and 1325 cribs in the 100-N Area to the Columbia River, (2) simulation of groundwater flow in operable unit 300-FF-5, (3) analysis of the T-106 single-shell tank release, and (4) preliminary analyses of liquid-effluent sites requested by EPA and the Washington State Department of Ecology (Ecology). VAM2DH has been used in support of solid waste disposal facility siting, and the purge water discharge analysis. TRACR3D has been used for unsaturated zone analysis in support of the grout facility. The actual transport modeling for this application was performed using S301 (Wikramaratna and Farmer 1987), a transport code that is designed for advective dominated transport applications; the code uses the velocity vectors from TRACR3D.

2.3.3.4 Saturated Zone Flow and Transport Model. Modeling of flow in the saturated sediments beneath the Hanford Site was initiated in the mid-1960's. During the late 1960's and 1970's the Hanford Site standard was represented by Variable Thickness Transient (VTT), a two-dimensional finite-difference groundwater flow computer code (Reisenauer 1979). Transport codes that used velocity vector output from VTT have also been developed. The TRANSS code (Simmons et al. 1986) has been applied to assess the potential transport of contaminants at various waste sites over the years on the Hanford Site. Results obtained using the VTT/TRANSS model were used in support of assessing the health risks associated with various Hanford Site defense waste scenarios evaluated in the HDW-EIS (DOE 1987).

During the early 1980's, the CFEST (Gupta et al. 1982) computer code was developed for use at the Hanford Site. For detailed combined flow and transport analyses, the CFEST computer code has replaced the VTT/TRANSS computer code. More recently, the MODFLO (USGS 1988), SLAEM (Strack 1989), and GGWP (GAI 1987) computer codes have been used to support various applications at the Hanford Site.

2.3.3.5 Multi-Phase Modeling. Development of multi-phase fluid flow and transport models was pioneered in the petroleum industry. Cases involving the disposal of volatile organic compounds that could migrate as separate fluid phases to the subsurface environment exist at locations on the Hanford Site. Experience in characterizing and modeling the fate and transport of these substances at the Hanford Site is limited. During fiscal year 1991, an investigation of a disposal site in the 200 Areas where large quantities of carbon tetrachloride have been disposed was initiated. Although the primary focus of this activity is to develop and test alternative methods for the purpose of characterizing and recovering large quantities of the carbon tetrachloride under the direction of an "expedited response action," an effort to apply existing computer codes and models to assist this effort was included in the scope of work. To date, emphasis has been placed on the use of PORFLO-3 to assist in this effort. Results from these preliminary analyses are not available. In addition to PORFLO-3, TRACR3D allows simulation of some aspects of multiphase flow. However, the use of TRACR3D in support of multi-phase modeling activities at the Hanford Site in unknown.

2.3.3.6 Geochemistry Modeling. Because of the importance of understanding and interpreting the geochemistry of natural waters, a number of chemical equilibrium computer codes have been developed in the last 20 years. Although these programs were originally research tools, they have become widely available and are commonly applied to a variety of hydrogeological problems. Even more so than the hydrogeological codes presented in this document, however, geochemical equilibria codes require the user to be quite knowledgeable. The user not only must be familiar with the specific details of these complex computer codes, but should also have a thorough understanding of the chemical processes that are being represented and the quality of the input data available.

Although a variety of geochemical codes have been used at the Hanford Site, only a small number have become mainstays for practical applications. Hanford Site experience with geochemical codes is related to their application in a wide variety of programs involving radioactive waste and hazardous chemicals. Some of the most common and widely accepted codes in use include: PHREEQE (Parkhurst et al. 1980); MINTEQ (Brown and Allison, 1987); EQ3, EQ6 (Wolery et al. 1990); and WATEQ (Ball et al. 1987). These codes have been modified to various extents over the last 10 years and a number of program versions are in existence. WATEQ has basic speciation of aqueous solutes capability, whereas MINTEQ, EQ3/EQ6, and PHREEQE have speciation and geochemical reaction sequencing capabilities. All of these computer codes are available for use in support of the RI/FS process.

3.0 SELECTION CRITERIA

3.1 ADMINISTRATIVE CRITERIA

Administrative criteria include availability, user support, useability, portability, modifiable, and reliability. It is believed that all the codes considered in this report satisfy the administrative criteria to some extent. Fulfillment of these administrative criteria will require support throughout the lifetime of the projects that rely on the selected computer codes. An explanation of each of these criteria is provided in the following sections.

3.1.1 Availability

Computer codes will be made available to all users for confirming modeling results. Generally speaking, public domain codes will be favored over proprietary software. However, the modeling committee believes that some proprietary software provided enhanced technical capability not available in existing nonproprietary software. The proprietary software included in the Hanford Site list of computer codes are required to have a licensing agreement that includes a mechanism for providing access to outside users wishing to examine the source code or run the executable code to confirm the Hanford Site modeling results. It is recognized that an excessive financial burden for such a licensing agreement could disqualify use of a code.

3.1.2 User Support

The primary criteria for selection will be that sufficient technical support will be available throughout the lifetime of the project from the software developer or distributor.

3.1.3 Useability

Useability refers to factors such as the ease of grid definition, parameter input, calibration, graphical capabilities, and the effectiveness of output presentation. Code documentation must be readily available and computer codes should be generally "user friendly." Computer codes currently in use at the Hanford Site have an established user community and are preferred over computer codes that are unfamiliar to Hanford Site users.

3.1.4 Portability

The software should operate on a variety of different hardware systems. A personal computer (PC) version is particularly desirable because PCs are more accessible.

3.1.5 Modifiable

Software modifications will likely be required to expand capabilities and allow inclusion of technological improvements. All modifications will be documented and controlled under computing software quality assurance guidelines.

3.1.6 Reliability

Quality assurance guidelines will include a testing program to verify all computer codes and validate models. Additionally, computer codes should have a history of effective use, with emphasis on Hanford Site usage.

3.2 TECHNICAL CRITERIA FOR CONCEPTUAL MODELS OF THE HANFORD SITE

This section describes the physical features and processes that are currently considered part of the Hanford Site conceptual transport models for air, surface water, and groundwater for conducting risk assessments. These conditions help define the technical capabilities considered in Section 3.3 and ultimately determine the criteria for the recommendations provided in Section 4.0.

3.2.1 Air Transport

During Hanford Site remediation, it is anticipated that various contaminants will become airborne. These contaminants could be released (continuous or instantaneous) in either gaseous or particulate form, or both. As contaminants are transported downwind, the concentration will be modified by three-dimensional dispersion, radioactive decay and chemical transformation, and gravitational deposition. The governing parameters describing these processes tend to be location and weather dependent; therefore, computer codes and models that have been demonstrated under Hanford Site conditions are considered most desirable. Based on current understanding, contaminant fate and transport analyses required to support risk assessments at the Hanford Site will likely be limited to individual sources located at ground level or a specified elevation. Multiple sources could be quantified using superposition. Additional requirements are likely if air transport becomes a major issue and more detailed analyses are required.

3.2.2 Surface Water Flow and Transport

Contamination could enter the Columbia River through diffusion, groundwater, influx, or direct discharge from seeps and springs. In either case, potential contamination is considered to be more of a localized problem than a regional problem due to the massive dilution capacity of the Columbia River. The average flow rate of the Columbia River in the Hanford Reach is approximately 3,000 cubic meters per second (DOE 1987), compared with an estimate of influx to the river over the entire Hanford Reach of approximately 1 cubic meter per second. This rate of influx is less than 0.04% of the Columbia River average flow rate.

Two specific needs for surface water flow and transport modeling have been identified, including: (1) prediction of river stage variation and its effect on contaminant migration near the Columbia River, and (2) downstream mixing of contaminants discharging from groundwater, springs, and seeps into the Columbia River. Modeling river stage variation will require quantification of the transient hydraulic behavior of the Columbia River in response to natural and man-made changes to the flow rate. Important factors may include the hydraulic profile of the river, bank storage, groundwater interactions, stream bed configuration, etc. Mixing of contaminants from groundwater, springs, and seeps discharging into the Columbia River will likely require modeling of point and distributed sources, advection, turbulent mixing (combining mass and momentum), and chemical partitioning between water and sediments. Additional factors may become important if surface water transport becomes a major issue and more detailed analyses are required.

3.2.3 Groundwater Transport

The transport of contaminants through the soil and groundwater of the Hanford Site sediments will require consideration of: (1) infiltration processes, (2) groundwater flow and transport of contaminants under partially saturated (vadose zone) conditions, and (3) groundwater flow and contaminant transport under saturated conditions.

3.2.3.1 Infiltration. Most of the waste at the Hanford Site is, and will be, contained in the vadose zone. Infiltration of water through these partially saturated sediments is considered the primary mechanism for release of waste to the accessible environment. As such, considerable emphasis has been placed on the study and quantification of the infiltration rate (i.e., the flux of water past the root zone). The physical processes that effect the infiltration rate include; precipitation, evaporation, transpiration, and drainage. Modeling infiltration at the Hanford Site requires the capability to simulate the following characteristics:

- Semiarid climate with average annual precipitation of 0.16 meters
- Temperatures in excess of 40°C, and extended periods of freezing temperatures
- Snow cover and snowmelt
- Evapotranspiration with little or no vegetation and variable rooting depths
- Layered soils with lithologies ranging from sand and gravel to sandy loam
- Simulation of groundwater flow under variably saturated conditions
- Soil heterogeneity; i.e., variations in hydraulic conductivity, storativity, effective and total porosity
- Soil heating and cooling.

3.2.3.2 Vadose Zone Flow and Transport. Once the water drains below the root zone, it is redistributed in the subsurface sediments. Drainage of water through these sediments is estimated to range from zero to 10 centimeters per year under natural conditions at the Hanford Site. Characteristics considered important for modeling vadose zone flow and transport at the Hanford Site are listed below:

- Moisture-dependent hydraulic conductivity relationships (characteristic curves) that differ for different soil types
- Hysteresis (characteristic curves that are dependent on the recent wetting and drying history of the soil)
- Vadose zone thickness ranging from several meters near the Columbia River to more than 20 meters beneath the 200 Area plateau
- Layered soils, including relatively impermeable caliche layers that may cause lateral spreading or perched water table conditions
- Discontinuous stratigraphic layers that are tilting in places
- First-order, linear sorption/desorption processes, using an effective distribution or retardation coefficient

- Radioactive decay.

Additional capabilities that may become important include: (1) heat transport, and (2) contaminant volatilization and vapor transport. In summary, a multi-dimensional, transient, partially saturated flow and transport modeling capability is required to simulate the behavior of contaminants in the vadose zone.

3.2.3.3 Saturated Flow and Transport. Contaminants transported through the vadose zone will become mixed with the groundwater in the unconfined aquifer. These contaminants will move with groundwater and could eventually reach downgradient pumping wells or the Columbia River. The flow velocity through the saturated sediments at the Hanford Site is estimated to range from several centimeters to several meters per day. Simulation of saturated groundwater flow and transport will be required to predict contaminant concentrations for use in support of risk assessments. Based on current understanding, saturated flow and transport modeling of Hanford Site conditions should account for the following conditions:

- Heterogeneous and isotropic porous media aquifer properties
- Layered soils with tilting beds in places
- Transient flow and transport behavior
- Confined and unconfined conditions
- Up to 70-feet variations in water table elevations with time, due to changes in waste-disposal practices at the Hanford Site, and future irrigation scenarios on or adjacent to the site
- Contaminant advection and dispersion
- Radiological and biological decay
- Contaminant retardation using an equilibrium sorption model with linear and completely reversible isotherms
- Point or distributed sources
- Aquifer/river interactions.

3.3 COMPARISON OF TECHNICAL CAPABILITIES

This section presents a matrix (Table 3-1) showing the modeling capabilities for each of the groundwater flow and transport computer codes considered for inclusion in the list of Hanford Site software. Only computer codes previously used at the Hanford Site were included in the matrix. The purpose of this matrix is to facilitate side-by-side comparison of the candidate software. Although air and surface water transport software were discussed in this report, none of these computer codes were eliminated from the list of Hanford Site software. Consequently, a matrix comparison of air and surface water transport software is not provided.

Table 3-1. Modeling Capabilities for Groundwater Flow and Transport Software.

Characteristic	UNSATH	PORFLO3	VAM2D	VAM3D	TRACR3D	S301	VTT	TRANSS	CFEST	GGWP	MODFLO	SLAEM
Confined Aquifer		X	X	X	X		X		X	X	X	X
Phreatic Aquifer[1]		X	X	X	X				X	X	X	
Heterogeneous Aquifer	X	X	X	X	X		X	X	X	X	X	X
Anisotropic K		X	X	X	X				X	X	X	
Single Fluid	X	X	X	X	X		X	X	X	X	X	X
Multiple Fluids		X			X							
Saturated		X	X	X	X		X	X	X	X	X	X
Unsaturated	X	X	X	X	X							
Transient Flow		X	X	X	X		X		X	X	X	X
Hysteresis			X									
Aquifer/River Interactions[2]											X	
Non-Orthogonal Grid				X					X	X		X
2-Dimensional (Horizontal)		X	X		X		X		X	X	X	X
2-Dimensional (Vertical)		X	X	X	X				X	X	X	
Pseudo 3-Dimensional[3]							X			X	X	X
3-Dimensional		X		X	X	X			X			
Advection/Dispersion[4]		X	X	X	X	X		X	X	X		
Linear Sorption		X	X	X	X	X		X	X	X		
Non-Linear Sorption												
Radioactive Decay		X	X	X	X	X		X	X	X		
Heat Transport	X	X							X			
Evapotranspiration	X		X	X								
Hanford Vegetation	X											

[1]Phreatic aquifer capability signifies that the aquifer transmissivity automatically adjusts to accommodate changes in the saturated thickness of the aquifer.
[2]Aquifer/river interactions refers to linking of a groundwater flow model and a streamflow routing model to simulate the interaction between groundwater and a dynamic river stage.
[3]Pseudo 3-dimensional refers to the capability to model layered aquifer systems without solving the fully three-dimensional system of equations, thereby reducing computational effort.
[4]TRANSS is a streamtube travel time model that does not actually solve the advection/dispersion equation.

4.0 RECOMMENDATIONS

Specific recommendations for computer codes included in the list of Hanford Site software are primarily dependent on the capability of the chosen software to simulate the majority of processes governing contaminant transport at the Hanford Site. A description of the most relevant processes, and comparison of the candidate groundwater codes to simulate these processes, were provided in the previous sections. The recommended codes and the rationale for their selection are provided in the following sections.

4.1 AIR

As stated in Section 2.4.1, it is recommended that simplified conservative analytical models be used whenever possible. These models have been encoded into several existing radiological safety codes used routinely at the Hanford Site (e.g., GENII [Napier et al. 1988]). With regard to GENII, two atmospheric transport models have been encoded; a straight line Gaussian model is used to compute acute maximum exposure based on an assumed maximum plume "centerline" concentration, and a chronic exposure model that assumes a sector-averaged concentration. The chronic exposure model also employs the use of the straight line Gaussian model for computing plume centerline concentrations. The source can either be released at ground level or at some elevation. Hanford Site meteorological conditions are programmed into GENII. Application of AIRDOS-PC will account for decreases in contaminant concentration resulting from deposition and scavenging. Similarly, if additional detail is required in the modeling of hazardous chemicals, it is recommended that the ISC computer code be applied.

4.2 SURFACE WATER

It is recommended that simplified conservative analytical models be used whenever possible. Guidance on the use of a one-dimension completely mixed model assuming the existence of a mixing zone is provided in EPA's Superfund Exposure Assessment Manual (EPA 1988). A solution to a quasi-two dimensional advective-dispersion model appropriate for estimating the decrease in contamination concentration resulting from lateral and longitudinal mixing is contained in GENII. Application of this analytical model should be more accurate but less conservative than application of the analysis methodology outlined in the EPA guidance document. If river stage variations resulting from hydropeaking and annual flooding is required, it is recommended that the DWOPER computer code, or equivalent, be applied. The DWOPER computer code has been applied by both the U.S. Army Corps of Engineers and the U.S. Bureau of Reclamation to simulate river stage variation in the Hanford Reach of the Columbia River (Fread 1973). Since the DWOPER computer code does not address sediment and sediment-related contaminant transport, if detailed analyses of these parameters are required to support future risk assessments based on information contained herein, it is recommended that the SERATRA (Onishi 1977) computer code or equivalent be applied. However, since the SERATRA computer code has not been used for several years, a review of currently available and maintained computer codes should be conducted prior to updating and implementing the SERATRA computer code.

4.3 GROUNDWATER FLOW AND TRANSPORT CODES

The recommended codes for the subsurface pathway include one infiltration code (UNSAT-H), two unsaturated zone codes (PORFLO-3 and VAM3D), and one saturated zone code (CFEST). The capabilities of these computer codes are outlined in the following sections, followed by a discussion of the rationale for choosing this set of codes.

4.3.1 UNSAT-H

UNSAT-H has been developed at the Hanford Site and is designed to simulate infiltration under typical Hanford Site conditions (Fayer and Jones 1990). UNSAT-H is a one-dimensional finite-difference code that accounts for precipitation, drainage, redistribution, evaporation, soil heating, and plant uptake of water. UNSAT-H allows specification of site-specific vegetation and soil conditions, and includes four different relationships between hydraulic conductivity and moisture content. The computer code will be used to establish moisture flux for the upper boundary condition in vadose zone flow and transport models. The code was selected because it best represents the current understanding on the quantification of those processes that govern infiltration at the Hanford Site.

4.3.2 PORFLO-3

PORFLO-3 (Sagar and Runchal 1990) is a fully three-dimensional, integrated finite-difference, flow and solute transport code with a wide variety of capabilities, including coupled unsaturated/saturated analysis, retardation, radioactive decay, and conductive heat transport. The geologic media may be heterogeneous and anisotropic and may contain linear and planar features such as boreholes and fractures. The computer code includes four different numerical solution techniques, each having certain advantages under differing conditions. Three options are available for specifying the relationship between hydraulic conductivity and moisture content. The computer code does not allow for hysteresis and is limited to grids with orthogonal geometry. PORFLO-3 has been applied at the Hanford Site, in addition to being developed (partially) at the Hanford Site. Although PORFLO-3 is proprietary, all use of the code in support of Hanford Site work is specifically excluded from the copyright limitation. Stochastic and multi-phase versions of PORFLO-3 are available.

PORFLO-3 was included in the list of Hanford Site software to simulate near-field unsaturated and saturated flow and transport in three dimensions. Although similar capabilities are available with VAM3D, PORFLO-3 was selected as the primary unsaturated flow and transport model for the following reasons:

- Westinghouse Hanford supported the development of this computer code for several years with the specific intention of using this computer code in support of environmental restoration activities

- The computer code has undergone extensive testing and peer review

- The code has been tailored to address the specific needs of the Hanford Site

- Hanford Site personnel have considerable experience in using this computer code

4.3.3 VAM3D

VAM3D (Huyakorn and Panday 1990) is a finite-element flow and solute transport code capable of coupled unsaturated/saturated analysis. Many of the features included in PORFLO-3 are included in VAM3D, although the VAM3D computer code cannot model heat flow. The code includes a routine for simulation of surface infiltration similar to UNSAT-H, although the infiltration routine is not specifically designed for the arid conditions found at the Hanford Site. Also, the aspect of hysteresis available in VAM2D can be easily incorporated into VAM3D. The code is proprietary; a licensing agreement will be modified to satisfy availability criteria.

VAM3D was included in the list of Hanford Site software because it utilizes a finite-element approach that will facilitate simulation of tilting and discontinuous bedding in the unsaturated zone. The computer code will also serve as a benchmark computer code for evaluating results obtained through the use of PORFLO-3. These intercode comparisons are considered extremely important during future testing of these computer codes.

In addition, the VAM3D computer code will be considered for area-wide saturated flow and transport analyses. As such, the VAM3D computer code has several capabilities that can be used in supporting environmental restoration activities.

4.3.4 CFEST

CFEST (Gupta et al. 1982) is a fully three-dimensional, finite-element, saturated flow and transport code developed at Pacific Northwest Laboratory. Capabilities include retardation and radioactive decay. The code was developed at Hanford for the Office of Nuclear Waste Isolation and the Seasonal Thermal Energy programs. As such, it was developed for confined aquifer systems and does not readily allow for changes in water table variation or changes in transmissivity resulting from water table variation. Recent proprietary versions have extended the capabilities of the CFEST computer code.

As stated previously, in the mid-1980's CFEST replaced the VTT/TRANSS computer code for performing detailed large-scale flow and transport analyses in the saturated sediments on the Hanford Site. As such, an operating version of the CFEST computer code is available for Hanford Site-wide application. However, this model has not been updated or applied fully at the Hanford Site for several years; therefore, user application of CFEST is unknown at this time. Based on discussions to date, it appears that the features of most importance, e.g., improved solver, adjustment of the water table, and transmissivity coefficients, have been developed and incorporated into the proprietary versions of the computer code. A licensing agreement does not exist for these versions in support of Hanford Site risk assessments.

It is recommended that CFEST be evaluated to support Hanford Site-wide risk assessments. This recommendation is based on the following considerations:

- An operational model of the Hanford Site saturated sediments that employs the use of CFEST exists
- The intrinsic value of using an integrated finite-element flow and transport computer code to model potential contaminant movement in the saturated sediments.

4.3.5 Summary

The four computer codes that have been selected for assessing contaminant fate and transport in the subsurface pathway (UNSAT-H, PORFLO-3, VAM3D, and CFEST) provide a broad base of analytical capability. Although some questions and concerns remain, it is believed that these computer codes, when appropriately implemented, will satisfy the administrative and technical criteria discussed in Section 3.0. In addition, this set of computer codes provides a level of technical redundancy considered prudent at this time based on current uncertainty. Although other codes are available for use in support of risk assessment, the selection reflects a "bias for action." As such, the computer codes that are currently is use in support of the Hanford Site remediation had a definite advantage.

4.4 SOFTWARE VERIFICATION AND BENCHMARKING

It is recommended that the computer codes in the list of Hanford Site software be verified and benchmarked against each other (when possible). Verification would involve inspection of the analytical formulation to confirm proper performance of the mathematical calculations and comparison of results against analytical solutions. In addition, the computer codes that have similar capabilities should be benchmarked under conditions typical of the Hanford Site to allow direct comparison. This process would develop an understanding of which codes are most appropriate for certain conditions and perhaps result in elimination of codes from the list of Hanford Site software. It is recommended that verification and benchmarking be initiated as soon as possible. If available, the results will be included in the second milestone (M-29-02).

4.5 FUTURE SOFTWARE APPROVAL PROCESS

As stated previously, the development of computer codes for modeling environmental pathways will continue to evolve. In the event that new or revised software is found to offer significant advantages, then its use in support of Hanford Site remediation activities will be considered. Two prerequisites for consideration of new software will be: (1) evidence of peer review and general acceptance by the technical community, and (2) recognition of the need for the additional software by the Hanford Site technical and regulatory communities. It is recommended that the software approval process will proceed in a manner similar to the selection of the computer codes contained herein, in that it would involve a committee of technical experts representing Ecology, EPA, and DOE. Since significant expansion of the list of Hanford Site codes is undesirable, additions of new codes to the list may require deletion of old codes. Alternatively, computer codes not included on the Hanford Site list may be approved for limited use in specialized applications.

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ATTACHMENT 2

TRANSMITTAL LETTER

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Department of Energy
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Mr. Paul T. Day
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Dear Messrs. Day and Nord:

HANFORD FACILITY AGREEMENT AND CONSENT ORDER MILESTONE M-29-01

This letters transmits copies of the "Description of Codes and Models to be used in Risk Assessment," DOE/RL-91-44, to complete the subject milestone. The milestone defines the document as a secondary document and requires submittal to the U.S. Environmental Protection Agency and State of Washington Department of Ecology by September 30, 1991.

If you have any questions, please call Mr. A. C. Harris at 509-376-4339.

Sincerely,

Steven H. Wisness
Hanford Project Manager

Enclosure

cc w/o encl.:
R. E. Lerch, WHC
T. B. Veneziano